```
C:\Program Files\Stnexp\Queries\038054.str
 \mathsf{CF}_3 \overline{\phantom{a}} [\mathsf{CF}_2]_{0-} [\mathsf{CH}_2]_{1-10}
chain nodes :
19 20 21 24 29 31 ring nodes:
                                                  38
```

```
19 20 21 24 29 31 38 39 45
ring nodes:
    1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds:
    2-24 5-29 9-31 12-38 14-39 17-45 19-20 20-21 21-24 29-31 38-39
ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
    15-16 16-17 17-18
exact/norm bonds:
    1-2 1-6 2-3 2-24 3-4 4-5 5-6 5-29 7-8 7-12 8-9 9-10 9-31 10-11 11-12 12-38
    14-39 17-45 19-20 20-21 21-24 29-31 38-39
normalized bonds:
    13-14 13-18 14-15 15-16 16-17 17-18
```

G1:C,O G2:C,O,N G3:C,O

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS 24:CLASS 29:CLASS 31:CLASS 38:CLASS 39:CLASS 45:CLASS

```
C:\Program Files\Stnexp\Queries\038054.str
    \begin{bmatrix} CF_2 \end{bmatrix}_{0-10} \begin{bmatrix} CH_2 \end{bmatrix}_{1-10}
chain nodes :
     19 20 21 24 29
                                    31
                                          38
                                               39
ring nodes:
1 2 3 4 chain bonds:
                       5 6
                                7
                                     8
                                          9 10 11
                                                          12
                                                                13
                                                                      14
                                                                            15
                                                                                   16
                                                                                         17
```

```
The first fields :

19 20 21 24 29 31 38 39

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

chain bonds :

2-24 5-29 9-31 12-38 14-39 19-20 20-21 21-24 29-31 38-39

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15

15-16 16-17 17-18

exact/norm bonds :

1-2 1-6 2-3 2-24 3-4 4-5 5-6 5-29 7-8 7-12 8-9 9-10 9-31 10-11 11-12 12-38

14-39 19-20 20-21 21-24 29-31 38-39

normalized bonds :

13-14 13-18 14-15 15-16 16-17 17-18
```

G3:C,O

Match level:

G1:C;O

G2:C,O,N

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS 24:CLASS 29:CLASS 31:CLASS 38:CLASS 39:CLASS

RN 225942-19-8 REGISTRY

ED Entered STN: 25 Jun 1999

CN Propanoic acid, 2-[[4'-(decyloxy)[1,1'-biphenyl]-4-yl]oxy]-,

3,3,4,4,5,5,6,6,6-nonafluorohexyl ester, (2R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C31 H37 F9 O4

CI COM

SR CA

Ring System Data

			Ring System		RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
========	+=======-	+===== = =		+=======-	-=======
C6	C6	6	C6	46.150.18	2

Absolute stereochemistry.

$$F_3C$$
 $(CF_2)_3$ O R O

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	11000000.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 4	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 7	(1) ACD
Bioconc. Factor (BCF)	1000000.0	8 Hq	(1) ACD
Bioconc. Factor (BCF)	1000000.0	рн 10	(1) ACD
Boiling Point (BP)	557.8+/-50.0 deg C		(1) ACD
Enthalpy of Vap. (HVAP)	83.97+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	280.4+/-45.0 deg C	j	(1) ACD
Freely Rotatable Bonds (FRB)	20		(1) ACD
H acceptors (HAC)	4		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	10000000.0	pH 1	(1) ACD
Koc (KOC)	10000000.0	pH 4	(1) ACD
Koc (KOC)	10000000.0	pH 7	(1) ACD
Koc (KOC)	10000000.0	8 Hq	(1) ACD
Koc (KOC)	10000000.0	pH 10	(1) ACD
logD (LOGD)	11.60	pH 1	(1) ACD
logD (LOGD)	11.60	pH 4	(1) ACD
logD (LOGD)	11.60	pH 7	(1) ACD
logD (LOGD)	11.60	pH 8	(1) ACD
logD (LOGD)	11.60	pH 10	(1) ACD
logP (LOGP)	11.598+/-0.889	ļ	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	< 0.01 mol/L	pH 4	(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1)	ACD
	<0.01 mol/L	рн 8	(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1)	ACD
Molecular Weight (MW)	644.61		(1)	ACD
Vapor Pressure (VP)	1.78E-12 Torr	25.0 deg C	(1)	ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

- L3 ANSWER 522 OF 682 REGISTRY COPYRIGHT 2004 ACS on STN
- RN 212779-64-1 REGISTRY
- ED Entered STN: 15 Oct 1998
- CN Benzoic acid, 4-[[4-[(7,7,8,8,9,9,9-heptafluorononyl)oxy]benzoyl]oxy]-, 4-[[(1-methylheptyl)oxy]carbonyl]phenyl ester (9CI) (CA INDEX NAME)
- FS 3D CONCORD
- MF C38 H41 F7 O7
- SR CA
- LC STN Files: CA, CAPLUS

Ring System Data

			Ring System		
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
========	}========	+== == ===-	+== ======+		
	1			46.150.18	•

F₃C-CF₂-CF₂-(CH₂)₆-0

PAGE 1-B

PROPERTY		VALUE	CONDITION	NO'	TE
Bioconc. Factor Bioconc. Factor Bioconc. Factor Bioconc. Factor Bioconc. Factor	(BCF) (BCF) (BCF) (BCF)	1000000.0 1000000.0 1000000.0 1000000.0 1000000.0	рН 1 рН 4 рН 7 рН 8 рН 10	(1) (1) (1)	ACD ACD ACD ACD ACD

Boiling Point (BP)	697.1+/-55.0 deg C	760.0 Torr	(1)	ACD
Enthalpy of Vap. (HVAP)	102.09+/-3.0 kJ/mol		(1)	ACD
Flash Point (FP)	361.2+/-47.5 deg C	į	(1)	ACD
Freely Rotatable Bonds (FRB)	23		(1)	ACD
H acceptors (HAC)	7	į	(1)	ACD
H donors (HD)	0	ĺ	(1)	ACD
Koc (KOC)	10000000.0	pH 1	(1)	ACD
Koc (KOC)	10000000.0	pH 4	(1)	ACD
Koc (KOC)	10000000.0	pH 7	(1)	ACD
Koc (KOC)	10000000.0	pH 8	(1)	ACD
	10000000.0	pH 10	(1)	ACD
	12.61	pH 1	(1)	ACD
_ !	12.61	pH 4	(1)	ACD
•	12.61	pH 7	(1)	ACD
logD (LOGD)	12.61	pH 8	(1)	ACD
logD (LOGD)	12.61	pH 10	(1)	ACD
	12.605+/-0.872		(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1)	ACD
	<0.01 mol/L	pH 4	(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1)	ACD
_	<0.01 mol/L	pH 8	(1)	ACD
-	<0.01 mol/L	pH 10	(1)	ACD
9	742.72	ļ	(1)	ACD
Vapor Pressure (VP)	2.78E-19 Torr	25.0 deg C	(1)	ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

- AN 131:163647 CA
- TI Synthesis, properties and crystal structure of chiral semiperfluorinated liquid crystals with ferro and anticlinic smectic phases
- AU Nguyen, H. T.; Rouillon, J. C.; Babeau, A.; Marcerou, J. P.; Sigaud, G.; Cotrait, M.; Allouchi, H.
- CS Centre de Recherche Paul Pascal, Universite de Bordeaux I, Pessac, 33600, Fr.
- SO Liquid Crystals (1999), 26(7), 1007-1019 CODEN: LICRE6; ISSN: 0267-8292
- PB Taylor & Francis Ltd.
- DT Journal
- LA English
- CC 75-11 (Crystallography and Liquid Crystals) Section cross-reference(s): 25, 74, 76
- An ew chiral and semiperfluorinated series with ferro and anticlinic properties was synthesized and characterized. The mesomorphic behavior was established on the grounds of both microscopic observations and DSC measurements. The nonchiral intermediate Et 4-semiperfluorinated alkyloxybenzoates exhibit SmA phases, unusual for compds. with a single Ph ring. The final derivs. display SmA, SmC* and in several cases SmCA* phases. The longer fluorinated chains favor the SmA and SmC* phases at the expense of the SmCA* phase. Electrooptical measurements were carried out with the classical SSFLC geometry. The spontaneous polarization and tilt angle at saturation are higher than those of the hydrogenous homologs, around 140 nC cm-2 at 40°. One compound of the series the 4,4,5,5,6,6,7,7,8,8,8-nonafluoroheptyloxy derivative crystallizes in the triclinic system, space group P1, with Z = 1 (4 mols./Z). The mols. are arranged in a head-to-tail fashion with two mols. oriented in the same direction and the two others in the opposite direction. They give rise to

sheets with a smectic C-like arrangement. The final reliability factors were R = 0.117 and WR = 0.134; the goodness of fit was S = 1.366.

methylheptyl fluorinated alkoxybenzoyloxybenzoyloxybenzoate prepn smectic liq crystal; mol structure methylheptyl fluoroheptyloxybenzoyloxybenzoylox ybenzoate; crystal structure methylheptyl fluoroheptyloxybenzoyloxybenzoyl oxybenzoate

IT Liquid crystals

> (antiferroelec.; synthesis, properties and crystal structure of chiral semiperfluorinated liquid crystals with ferro and anticlinic smectic phases)

IT Liquid crystals

> (ferroelec.; synthesis, properties and crystal structure of chiral semiperfluorinated liquid crystals with ferro and anticlinic smectic phases)

TT Antiferroelectric materials

Ferroelectric materials

(liquid-crystal; synthesis, properties and crystal structure of chiral semiperfluorinated liquid crystals with ferro and anticlinic smectic phases)

Crystal structure IT

Molecular structure

(of methylheptyl nonafluoroheptyloxybenzoyloxybenzoyloxybenzoate)

IT Electrooptical effect

Phase transition enthalpy

(of methylheptyl semiperfluorinated alkoxybenzoyloxybenzoyloxybenzoate liquid crystals)

ΙŤ Liquid crystals

> (smectic A; preparation and properties of Et semiperfluorinated alkyloxybenzoates and methylheptyl semiperfluorinated alkoxybenzoyloxybenzoyloxybenzoates)

IT Liquid crystals

(smectic; preparation and phase behavior of methylheptyl semiperfluorinated alkoxybenzoyloxybenzoyloxybenzoates)

IT Ferroelectricity

> (spontaneous polarization; of methylheptyl semiperfluorinated alkoxybenzoyloxybenzoyloxybenzoate liquid crystals)

IT 237754-96-0P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(preparation and crystal structure and liquid-crystal properties of)

IT212779-64-1P 237754-87-9P 237754-88-0P 237754-89-1P 237754-90-4P 237754-91-5P 237754-93-7P 237754-92-6P 237754-94-8P 237754-95-9P 237754-97-1P 237754-98-2P 237754-99-3P 237755-01-0P 237755-03-2P 237755-04-3P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (preparation and liquid crystal properties of)

IT 212779-66-3P

> RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (preparation and liquid-crystal and electrooptic properties of)

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD 25

- RE.CNT (1) Anon; International Tables for X-Ray Crystallography 1974, VIV
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- (3) Chandani, A; Jpn J appl Phys 1989, V28, P1261
- (4) Doi, T; J mater Chem 1991, V1, P169 CAPLUS
- (5) Drzewinski, W; Proceedings of the 6th International Conference on FLCs 1997, P156
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- (7) Goodby, J; Nature 1989, V337, P449 CAPLUS
- (8) Ivashenko, A; Mol Cryst liq Cryst 1981, V67, P235
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- (10) Kromm, P; Acta Cryst 1995, VC51, P1229 CAPLUS (11) Kromm, P; Liq Cryst 1996, V21, P121 CAPLUS

```
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(15) Liu, H; Liq Cryst 1997, V22, P217 CAPLUS
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(18) Nguyen, H; Liq Cryst 1991, V10, P389
(19) North, A; Acta Cryst 1968, VA24, P351
(20) Pucci, D; Liq Cryst 1996, V21, P153 CAPLUS
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    1993
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(24) Tournilhac, F; Ferroelectrics 1991, V114, P283 CAPLUS
(25) Twieg, R; SPIE 1991, V1455, P86
REFERENCE 2
AN
     129:237922 CA
ΤI
     Dielectric, optical and TSM measurements on semi-perfluoro ferro- and
     antiferroelectric liquid crystals
ΑU
     Sarmento, S.; Carvalho, P. Simeao; Glogarova, M.; Chaves, M. R.; Nguyen,
     H. T.; Ribeiro, M. J.
CS
     Departamento de Fisica, IMAT (nucleo IFIMUP), CFUP, Faculdade de Ciencias
     da Universidade do Porto, Oporto, 4150, Port.
     Liquid Crystals (1998), 25(3), 375-385
SO
     CODEN: LICRE6; ISSN: 0267-8292
PB
     Taylor & Francis Ltd.
DT
     Journal
LΑ
     English
CC
     75-11 (Crystallography and Liquid Crystals)
     Section cross-reference(s): 73, 76
AB
     Two compds. with very similar chemical formulas but different phase sequences
     F3H6 and F4H6, where FnHm = CnF2n+1-CmH2mO-C6H4-COO-C6H4-COO-C6H4-
     COOCH(Me)-C6H13,, were studied by dielec., optical and TSM (temperature scan
     method) measurements, and by optical and polarization hysteresis loops.
     The light diffraction technique was used to measure the helical pitch (p),
     which is nearly temperature independent. Six relaxation modes were identified.
     The polarization and tilt angle results are discussed using a simple
     phenomenol. model and fitted to the equation P0/00 \approx
     (1/\epsilon\epsilon0C - (\Omega/C)\theta02)-1. The parameters C and
     \Omega were determined from the fitting.
     fluorinated ferroelec antiferroelec liq crystal dielec; polarization
ST
     spontaneous fluorinated ferroelec antiferroelec mesophase; helical pitch
     fluorinated ferroelec antiferroelec mesophase; phase sequence fluorinated
     ferroelec antiferroelec mesophase; relaxation frequency fluorinated
     ferroelec antiferroelec mesophase
IT
     Liquid crystals
        (antiferroelec.; dielec., optical and temperature scan method measurements
on
        semi-perfluoro)
```

IT Liquid crystals

(ferroelec.; dielec., optical and temperature scan method measurements on semi-perfluoro)

IT Antiferroelectric materials Ferroelectric materials

(liquid-crystal; dielec., optical and temperature scan method measurements

semi-perfluoro)

١

IT Dielectric constant
Dielectric relaxation
Electrooptical effect

(of semi-perfluoro ferro- and antiferroelec. liquid crystals)

IT Ferroelectricity

on

(spontaneous polarization of semi-perfluoro ferro- and antiferroelec. liquid crystals)

IT 212779-66-3

RL: PRP (Properties)

(dielec., optical and temperature scan method measurements on semi-perfluoro ferro- and antiferroelec. liquid crystals)

IT 212779-64-1

RL: PRP (Properties)

(dielec., optical and temperature scan method measurements on semi-perfluoro ferroelec. liquid crystals)

- RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
- (1) Carlsson, T; Phys Rev A 1990, V42, P877 CAPLUS
- (2) Carvalho, P; Liq Cryst 1996, V21, P115 CAPLUS
- (3) Carvalho, P; Liq Cryst 1996, V21, P511
- (4) Destrade, C; Ferroelectrics 1996, V177, P161 CAPLUS
- (5) Faye, V; Liq Cryst 1995, V19, P47 CAPLUS
- (6) Fukuda, A; J Mater Chem 1994, V4, P997 CAPLUS
- (7) Fukui, M; Jpn J appl Phys 1990, V29, P329
- (8) Goodby, J; Ferroelectric Liquid Crystals-Principles Properties and Applications, Vol 7, Ferroelectricity and Related Phenomena 1991
- (9) Levstik, A; Phys Rev A 1987, V35, P3527 CAPLUS
- (10) Lines, M; Principles and Applications of Ferroelectrics and Related Materials 1977
- (11) Nguyen, H; To be published
- (12) Novotna, V; Liq Cryst 1997, V23, P511 CAPLUS
- (13) Uehara, H; Jpn J appl Phys 1995, V34, P5424 CAPLUS

RN 225942-19-8 REGISTRY

ED Entered STN: 25 Jun 1999

CN Propanoic acid, 2-[[4'-(decyloxy)[1,1'-biphenyl]-4-yl]oxy]-,

3,3,4,4,5,5,6,6,6-nonafluorohexyl ester, (2R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C31 H37 F9 O4

CI COM

SR CA

Ring System Data

			Ring System		RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
========	+=======	+==== ==	}=========	}========	- -=========
C6	C6	6	C6	46.150.18	2

Absolute stereochemistry.

$$F_3C$$
 $(CF_2)_3$ O R O $CH_2)_9$ Me

PROPERTY (CODE)	VALUE	CONDITION	NOTE
=======================================	+============	+========	
Bioconc. Factor (BCF)	1000000.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 4	(1) ACD
Bioconc. Factor (BCF)	1000000.0	рн 7	(1) ACD
Bioconc. Factor (BCF)	1000000.0	8 Hq	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 10	(1) ACD
Boiling Point (BP)	557.8+/-50.0 deg C	~	(1) ACD
Enthalpy of Vap. (HVAP)	83.97+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	280.4+/-45.0 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	20		(1) ACD
H acceptors (HAC)	4		(1) ACD
H donors (HD)	О		(1) ACD
Koc (KOC)	10000000.0	pH 1	(1) ACD
Koc (KOC)	10000000.0	pH 4	(1) ACD
Koc (KOC)	10000000.0	pH 7	(1) ACD
Koc (KOC)	10000000.0	8 Hq	(1) ACD
Koc (KOC)	10000000.0	pH 10	(1) ACD
logD (LOGD)	11.60	pH 1	(1) ACD
logD (LOGD)	11.60	pH 4	(1) ACD
logD (LOGD)	11.60	pH 7	(1) ACD
logD (LOGD)	11.60	PH 8	(1) ACD
logD (LOGD)	11.60	pH 10	(1) ACD
logP (LOGP)	11.598+/-0.889	~	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD

Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	рн 8	(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1)	ACD
Molecular Weight (MW)	644.61		(1)	ACD
Vapor Pressure (VP)	1.78E-12 Torr	25.0 deg C	(1)	ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

[]3/a]

RN	479201-31-5	REGISTRY

ED Entered STN: 16 Jan 2003

CN Oxiranecarboxylic acid, 3-propyl-, 4-[5-[(5,5,6,6,7,7,8,8,8-nonafluorooctyl)oxy]-2-pyrimidinyl]phenyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H23 F9 N2 O4

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
========	+=======	+=======	+==========	+========	+=======
C20	OC2	3	C20	1.30.1	1
C6	C6	6	C6	46.150.18	1
C4N2	NCNC3	ĺ 6	C4N2	46.195.39	11

Relative stereochemistry.

PROPERTY (CODE)	VALUE	CONDITION	NOTE
PROPERTY (CODE) ===================================	VALUE +====================================	pH 1 pH 4 pH 7 pH 8 pH 10 760.0 Torr	(1) ACD (1) ACD (1) ACD (1) ACD (1) ACD (1) ACD
Freely Rotatable Bonds (FRB) H acceptors (HAC) H donors (HD) Koc (KOC) Koc (KOC) Koc (KOC) Koc (KOC) Koc (KOC)	14 6 0 11270 22376 22398 22398 22398	рн 1 рн 4 рн 7 рн 8 рн 10	(1) ACD (1) ACD (1) ACD (1) ACD (1) ACD (1) ACD (1) ACD (1) ACD

logD (LOGD)	5.17	pH 1	(1)	ACD
logD (LOGD)	5.47	pH 4	(1)	ACD
logD (LOGD)	5.47	рн 7	(1)	ACD
logD (LOGD)	5.47	рн 8	(1)	ACD
logD (LOGD)	5.47	pH 10	(1)	ACD
logP (LOGP)	5.467+/-1.234		(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1)	ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1)	ACD
Molecular Weight (MW)	574.44		(1)	ACD
pKa (PKA)	0.99+/-0.20	Most Basic	(1)	ACD
Vapor Pressure (VP)	5.13E-10 Torr	25.0 deg C	(1)	ACD
•				

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:64125 CA

TI Liquid crystalline materials containing perfluoroalkyl and alkenyl tail groups

IN Gough, Neil; Vohra, Rohini; Wand, Michael; More, Kundalika; Thurmes, William N.

PA USA

SO U.S. Pat. Appl. Publ., 46 pp.

CODEN: USXXCO

DT Patent

LA English

IC ICM C09K019-34

ICS C09K019-32; C09K019-30; C09K019-20; C09K019-12; C07D239-02

NCL 252299610

CC 75-11 (Crystallography and Liquid Crystals)

FAN.CNT 1

PATENT NO.		KIND	DATE	APPLICATION NO.	DATE	
ΡI	US 2002195585	A1	20021226	US 2001-754034	20010103	

PRAI US 2000-255984P 20001215

This invention describes compds. that are useful as components in liquid crystal compns., particularly in ferroelec. liquid crystal compns. Compds. of the invention are rod-like mols. with a mesogenic (generally linear) core to which an alkene tail and an alkyl or alkoxy tail with a perfluoroalkyl terminal portion are bonded. Compds. of the invention can contain a variety of 1, 2 or 3 ring cores, wherein the rings maybe aromatic or alicyclic. Alkenes of the invention are useful as components to improve LC properties of mixts., for example, to lower m.p. or to lower f.p., of LC compns.

ST ferroelec liq crystal perfluoroalkyl alkenyl tail group

IT Liquid crystals

(ferroelec.; liquid crystalline materials containing perfluoroalkyl and alkenyl

tail groups)

IT Ferroelectric materials

(liquid-crystal; liquid crystalline materials containing perfluoroalkyl and alkenyl

tail groups)

IT Liquid crystals

(nematic; liquid crystalline materials containing perfluoroalkyl and alkenyl tail

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groups)
IT
     Liquid crystals
        (smectic; liquid crystalline materials containing perfluoroalkyl and
alkenyl tail
        groups)
IT
     479201-26-8P
     RL: SPN (Synthetic preparation); TEM (Technical or engineered material
     use); PREP (Preparation); USES (Uses)
        (liquid crystalline materials containing perfluoroalkyl and alkenyl tail
groups)
IT
     57202-38-7
                  57202-39-8
                               57202-48-9
                                             57202-54-7
                                                          57202-58-1
     120091-49-8
                   121083-93-0
                                 121218-85-7
                                                121218-90-4
                                                              121235-87-8
     126162-76-3
                   126163-69-7
                                  155468-60-3
                                                308107-81-5
                                                              402860-34-8
     439866-35-0
                   460359-38-0
                                  460359-39-1
                                                460359-40-4
                                                              460359-42-6
     460359-43-7
                   460359-44-8
                                 460359-45-9
                                                460359-51-7
                                                              479201-27-9
     479201-28-0
                   479201-29-1
                                 479201-30-4
                                                479201-31-5
                                                              479201-32-6
     479201-33-7
                   479201-34-8
                                 479201-35-9
                                                479201-36-0
                                                              479201-37-1
     479201-38-2
     RL: TEM (Technical or engineered material use); USES (Uses)
        (liquid crystalline materials containing perfluoroalkyl and alkenyl tail
groups)
IT
     2108-05-6, trans-3-Hepten-1-ol
                                      2695-48-9, 8-Bromo-1-octene
                                                                     20125-84-2
     56578-18-8, trans-5-Decen-1-ol
                                       64275-73-6
                                                    460359-29-9
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis of liquid crystalline materials containing perfluoroalkyl and
alkenyl
        tail groups)
IT
     479201-23-5P
                    479201-24-6P
                                   479201-25-7P
     RL: SPN (Synthetic preparation); TEM (Technical or engineered material
     use); PREP (Preparation); USES (Uses)
        (synthesis of liquid crystalline materials containing perfluoroalkyl and
alkenyl
        tail groups)
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